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Modeling of Etching Nano-surfaces of Indium Phosphide

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This paper describes a mechanism for obtaining a regular porous structure InP, which is to use the method of photoelectrochemical etching. Through the use of simulation etching at the nanoscale, it is possible to get a regular uniform grid of nanopores on the surface of indium phosphide, which allows us to understand the mechanisms and the establishment of technological regimes anodic structures indium phosphide to produce a variety of devices.

Keywords: InP, Porous, Modeling, Nano-surfaces.

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1. INTRODUCTION

Indium phosphide – a technologically important material for the development of lasers, diodes, solar cells. At present, special attention is paid to properties of the porous InP, since it is a very important material for producing light-emitting diodes and solar cells. This paper describes a mechanism for obtaining a regular porous structure InP, which is to use the method of photoelectrochemical etching. Through the use of simulation etching at the nanoscale, it is possible to get a regular uniform grid of macropores on the surface of indium phosphide, which allows us to understand the mechanisms and the establishment of technological regimes anodic structures indium phosphide to produce a variety of devices.

Made in the recent progress in the study of the properties of porous silicon has stimulated similar studies for semiconductor compounds AIIIBV. In particular, the most promising in this aspect is the porous InP, as the energy parameters of its single crystals are very close to the parameters of single crystal silicon and on the basis thereof the device is easy to manufacture integrated optoelektronika compatible with silicon, in particular the resistive and the optocoupler diode.

As the electrolyte for producing porous materials AIIIBV (in particular InP) may use the halide, sulfate, phosphate, nitrate, water and non-aqueous solutions of alkalis at significant current densities, [1-6]. In most cases, the electrolytic etching of binary compounds AIIIBV must be used HCl in ethanol or water.

Indium phosphide anisotropy manifests itself not only in the general physical properties, but also during digestion crystal. Anisotropic etching is important for the structuring of semiconductors and is mainly due to differences in the rate of digestion of low indexed surfaces of crystals. The reasons for this behavior are not yet fully understood. Typically, we investigate low-indexed crystal surface – this orientation (111), (100), (110) [7, 8].

2. RESULTS AND DISCUSSION

Consider the process of dissolution of the electrode, the thickness of which is comparable to or less than the diffusion length of holes. In this case, it is necessary to take into account the processes occurring on the ohmic contact.

For definiteness, we consider further *n*-type semiconductor.

To find the value of the limiting current of the anodic dissolution consider the motion of holes in the quasi-neutral region.

Condition for the preservation of the holes is expressed as follows:

$$\frac{\partial p(x)}{\partial t} = -\frac{p(x)-p^0}{\tau_P} - \frac{1}{e}\frac{d}{dx} i_P(x) \qquad (1)$$

where $i_P(x)$ and $p(x)$ – respectively the hole current and the concentration of holes at the point x; τ_P – hole lifetime.

The first term in accordance with the process described recombination – generation of holes. The second – to change the current coordinate, which means that the flow of holes included in the unit volume of the semiconductor, is not equal to the flux flowing out of it.

The difference between these flows is determined by varying the concentration of holes in time. Thus, the ratio of (1) establishes a balance hole.

Since the quasi-neutral region is not charged, and the electric field in it is small, the minority carriers move by diffusion mechanism, and the current $i_P(x)$ can be written as:

$$i_P(x) = -eD_P\, dp/dx \qquad (2)$$

Let the distance $x = L$ from the boundary InP – electrolyte is an ohmic contact with the semiconductor metal. We characterize the contact surface recombination velocity s.

Solution of the continuity equation for holes can be written as:

$$p = p^0 + Ae^{-\frac{x}{L_P}} + Be^{\frac{x}{Lp}} \qquad (3)$$

To find the constants A and B need to formulate two boundary conditions. The first condition.

Assume that the hole current flowing through the ohmic contact is given by:

$$i_P(L) = -es\left[p(L) - p^0 \right] \quad (4)$$

where $p(L)$ – the concentration of holes in the plane of the ohmic contact.

The second condition

$$p(x = L_1) = 0 \quad (5)$$

obtain the relation

$$e\frac{D_P}{L_P}\left[-Ae^{-\frac{L}{L_P}} + Be^{\frac{L}{L_P}} \right] = es\left[p(L) - p^0 \right] \quad (6)$$

Equation (5) can be written using the formula (3)

$$p^0 + A + B = 0 \quad (7)$$

Solving the system of equations (6) and (7) we find that A and B

$$A = -p^0 - \frac{p^0}{2}\frac{se^{\frac{-L}{L_P}} - D_P L_p^{-1} e^{-\frac{L}{L_P}}}{D_P L_P^{-1} ch\frac{L}{L_P} + s \cdot sh\frac{L}{L_P}} \quad (8)$$

$$B = \frac{p^0}{2}\frac{se^{\frac{-L}{L_P}} - D_P L_p^{-1} e^{-\frac{L}{L_P}}}{D_P L_P^{-1} ch\frac{L}{L_P} + s \cdot sh\frac{L}{L_P}} \quad (9)$$

The current limit is

$$i_p^{npe\partial} = -eD_P \left.\frac{dp}{dx}\right|_{x=0} = -\frac{eD_P}{L_P}(-A + B) \quad (10)$$

As one cell structure has been selected, as shown in Fig. 1.

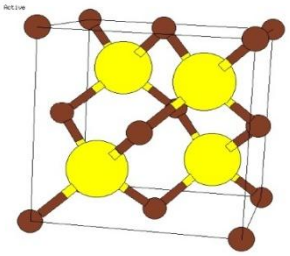

Fig. 1 – Structure of the cell InP

Nanostructure was simulated by computer merging cells InP (Fig. 1) in height, width and thickness. Then at the reference distance has been selected point of interaction with the surface intended for current flow etching. The current value is calculated by the proposed calculation and should not exceed this value. Parameters for calculating wondered existing publication of the results of different authors. Thus the result is a visual representation of the possible appearance of nanopores in the etching of indium phosphorus.

Modeling of etching provided for the reaction from the top to the bottom. The figure shows the red lines, where the contacts for the current flow. The simulation was performed under the condition to obtain a porous structure of satisfactory quality just by using hydrochloric acid (concentration of not less than 5 %) at a current density of 100-200 mA/cm2, and etching time of 15 to 30 minutes.

For the simulation program was developed in the programming language C++. The result of which was obtained by the file. To view the file used the program RasWin Molecular Grafics Windows Version 2.6.

3. CONCLUSION

Simulation result was obtained on the surface of the nanopore indium phosphide (Fig. 2), which clearly shows the mechanism of formation of nanoporous structure of indium phosphide. It should be noted that when trawling the n-type formation of the porous structure is observed at different concentrations of electrolyte, time, current density.

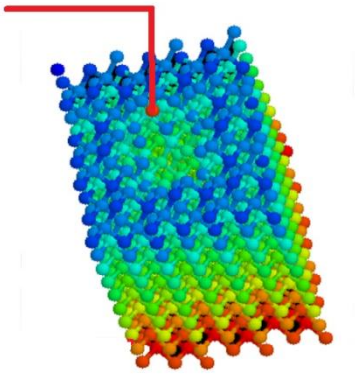

Fig. 2 – Nanopore structure of indium phosphide (cell structure 7 × 7 × 10)

One of the reasons for determining differences different crystallographic planes may be the density of atoms in these crystallographic planes (high density = low dissolution rate). However, this is not the only factor determining the anisotropy. In III-V compounds, there are several additional factors that contribute to anisotropy is due to the different chemical properties of atoms in the third and fifth groups of the periodic table of elements. For example, along the surface orientation <111> atomic plane occupied by atoms of the third and fifth groups form double layers that are small and large gaps between the planes {111}, alternating. Each atom has 3 bonds within a double layer and a connection outside the double layer.

Surfaces In limited atoms called {111A}, while limited atoms P – {111B} important to note that almost all surface oxidation processes of type {111} have slower dissolution rate. This can be explained by assuming that the three services (within the same double layer) is much harder to break from A than from B, due to the fact that the electron cloud of one connection is polarized in the direction of B atom (more electronegative).

Represented by the surface morphology of the porous n-InP (Fig. 3) produced by electrochemical etching in 5 % HCl, a current density of 80 mA/cm² , the etching time is 5min. More detailed information can be found in our paper [9].

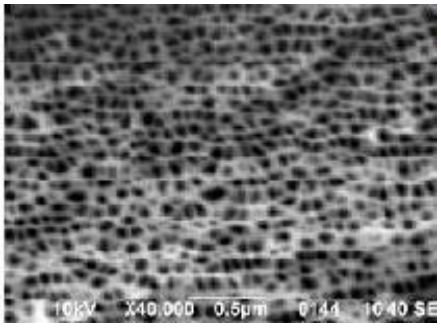

Fig. 3 – Surface morphology of the porous n-InP

ACKNOWLEDGMENT

The size of the pores in the visual simulation of etching the surface of the nano-structure of indium phosphide were approximately 10-60 nm, the porosity of 20-42 %. It's time boosted by deep into the structure. The parameters that allow us to state

In our opinion, these pores are due to the appearance of the output of the crystal surface dislocations and micro-defects, the place of origin which are favorable for the formation of pores.

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